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Rietveld, Cation Distribution and Elastic Investigations of

Nanocrystalline Li_{0.5+0.5x}Zr_xFe_{2.5-1.5x}O₄ Synthesized via Sol-gel Route

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Abstract

The present report deals with the structural and elastic behavior of Li⁺ and Zr⁴⁺ substituted

spinel ferrites. Nanocrystalline spinel ferrite system of chemical formula Li_{0.5+0.5x}Zr_xFe_{2.5-}

 $_{1.5x}O_4$ (where, x = 0.0, 0.1, 0.2, 0.3, 0.4, 0.5 and 0.6) was synthesized by using sol-gel auto

combustion method. The as-prepared powder was annealed at 800 °C for 5 h for better

crystallinity. The annealed samples were characterized by X-ray diffraction technique and

Fourier transform infrared spectroscopy for structural and elastic studies respectively. By

applying the full pattern fitting of Rietveld method the x, y, z coordinates of atoms, unit cell

dimensions and occupancy of ions were estimated. The lattice parameter was found to

decrease after substitution due to increase in electron affinity. Site preferences of cations

were obtained by matching experimental and calculated intensity. The characteristic bands of

crystallographic sub-lattice for the cubic structure were observed by FTIR spectra.

Keywords: Li-Zr ferrite; Rietveld; Spinel; Cation distribution; Elastic properties.

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1

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